

Multiplicativity in the theory of coincidence site lattices

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Abstract. Coincidence Site Lattices (CSLs) are a well established tool in the theory of grain boundaries. For several lattices up to dimension $d = 4$, the CSLs are known explicitly as well as their indices and multiplicity functions. Many of them share a particular property: their multiplicity functions are multiplicative. We show how multiplicativity is connected to certain decompositions of CSLs and the corresponding coincidence rotations and present some criteria for multiplicativity. In general, however, multiplicativity is violated, while supermultiplicativity still holds.

1. Introduction

In crystallography CSLs have been used for several decades to classify and describe grain boundaries, see e.g. [1–4] and references therein. In the beginning research concentrated on lattices in dimensions $d \leq 3$, but since the discovery of quasicrystals also lattices in higher dimensions and \mathbb{Z} -modules have been studied, see e.g. [4–6]. Here we discuss a special aspect, namely the multiplicativity of certain combinatorial functions associated with CSLs.

Let us recall some basic concepts. Let $\Gamma \subseteq \mathbb{R}^d$ be a d -dimensional lattice and $R \in O(d)$ a linear isometry. Then, R is called a (linear) *coincidence isometry* of Γ if $\Gamma(R) := \Gamma \cap R\Gamma$ is a lattice of finite index in Γ , and $\Gamma(R)$ is called an (ordinary or simple) *coincidence site lattice (CSL)* (for an introduction, see [4]). The group of all coincidence isometries of Γ is denoted by $OC(\Gamma)$, whereas the subgroup of all orientation preserving isometries is called the group of coincidence rotations and referred to as $SOC(\Gamma)$. The *coincidence index* $\Sigma(R) := [\Gamma : \Gamma(R)]$ is defined as the (group theoretical) index of $\Gamma(R)$ in Γ and is just the ratio of the volume of the corresponding unit cells.

These concepts can be generalized to include the possibility of multiple CSLs, see [7–9]. In particular, the lattice

$$\Gamma(R_1, \dots, R_n) := \Gamma \cap R_1\Gamma \cap \dots \cap R_n\Gamma = \Gamma(R_1) \cap \dots \cap \Gamma(R_n) \quad (1)$$

is called a *multiple CSL (MCSL)* of order n , where R_i , $i \in \{1, \dots, n\}$, are coincidence isometries of Γ . Its index in Γ is denoted by $\Sigma(R_1, \dots, R_n)$.

There arise several interesting combinatorial questions in this context. In particular, one is interested in the number of coincidence isometries, coincidence rotations and the number of CSLs of a given index m , which we denote by $|\mathcal{P}|f^{iso}(m)$, $|\mathcal{P}'|f^{rot}(m)$ and $f(m)$, respectively. Here $|\mathcal{P}|$ is the order of the point group \mathcal{P} of Γ , and $\mathcal{P}' \subseteq \mathcal{P}$ is the (normal) subgroup of orientation

preserving symmetry operations. These factors have been chosen to guarantee that $f^{iso}(m)$ and $f^{rot}(m)$ are normalized such that $f^{iso}(1) = 1$ and $f^{rot}(1) = 1$, respectively. In general we have $f^{iso}(m) \geq f(m)$, although $f^{iso}(m) = f^{rot}(m) = f(m)$ holds for the most important examples in $d = 2, 3$ like the square lattice and the cubic lattices. In $d \geq 4$ there exist several examples where $f^{iso}(m) = f^{rot}(m) > f(m)$ for infinitely many indices m , see e.g. [10, 11] for examples.

In many cases the multiplicity functions $f^{iso}(m)$, $f^{rot}(m)$ and $f(m)$ turn out to be multiplicative functions. Recall that a function $f : \mathbb{N} \rightarrow \mathbb{R}$ is called multiplicative if $f(mn) = f(m)f(n)$ holds whenever m and n are coprime. We call f supermultiplicative if the inequality $f(mn) \geq f(m)f(n)$ holds for m and n coprime. As an example we mention the square lattice [4], where

$$f^{iso}(m) = f^{rot}(m) = f(m) = \begin{cases} 1 & \text{for } m = 1 \\ 2^r & \text{if all prime factors } p \text{ of } m \text{ satisfy } p \equiv 1 \pmod{4} \\ & \text{and } r \text{ is the number of distinct prime factors} \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

Multiplicativity suggests to use a Dirichlet series as generating function, which reads in this case [4]

$$\begin{aligned} \Phi(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} = \prod_{p \equiv 1(4)} \frac{1 + p^{-s}}{1 - p^{-s}} \\ &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \dots \end{aligned} \quad (3)$$

Note that it is the multiplicativity of $f(m)$ that guarantees that the product expansion exists. In case of the square lattice, multiplicativity is a consequence of the fact that $\mathbb{Z}[i]$ is a principal ideal domain. But multiplicativity also holds for the cubic lattices in 3 dimensions as well as for the A_4 root lattice and the hypercubic lattices in 4 dimensions [4, 10, 12]. In the latter cases multiplicativity is due to the unique prime factorization in certain quaternion algebras.

All these cases are quite special in the sense that they are related to algebras that allow a unique prime factorization. In fact, there are examples where $f(m)$ and $f^{iso}(m)$ are not multiplicative, e.g. for $\Gamma = 2\mathbb{Z} \times 3\mathbb{Z}$. This raises several questions: when are the multiplicity functions multiplicative, are there criteria for multiplicativity? Does the multiplicativity of $f(m)$ imply the multiplicativity of $f^{iso}(m)$ or $f^{rot}(m)$ or vice versa? Is there a connection between the multiplicativity of the multiplicity functions for ordinary CSLs and multiple CSLs? What can be said if $f(m)$ is not multiplicative?

We answer some of these questions below and show that there are some connections between multiplicativity and certain decompositions of CSLs into multiple CSLs. We explain and motivate our results and sketch some proofs, whereas detailed proofs will be published elsewhere.

For simplification we will consider only $f^{iso}(m)$ and $f(m)$ in the following. In fact, this is no restriction since all properties of $f^{iso}(m)$ have a direct counterpart for $f^{rot}(m)$. Moreover $f^{rot}(m) = f^{iso}(m)$ for all lattices Γ that contain an orientation reversing symmetry operation in their point group, since there exists an index preserving bijection between the symmetry preserving and symmetry reversing coincidence isometries — compare the remark at the beginning of Sec. 3 of [12].

2. Multiplicativity and supermultiplicativity of the coincidence index

Before looking at the multiplicity functions $f(m)$, it makes sense to have a closer look on the coincidence index $\Sigma(R)$. In particular we are interested in $\Sigma(R_1 R_2)$, if R_1 and R_2 are coincidence isometries. We cannot expect to calculate $\Sigma(R_1 R_2)$ from $\Sigma(R_1)$ and $\Sigma(R_2)$, but we get at least the following upper bound:

Lemma 1. $\Sigma(R_1 R_2)$ divides $\Sigma(R_1) \Sigma(R_2)$.

The proof makes use of the second homomorphism theorem and can be deduced from the diagram in Fig. 1, which shows the relation of several CSLs and double CSLs. There we have set $m := \Sigma(R_1)$ and $n := \Sigma(R_2)$.

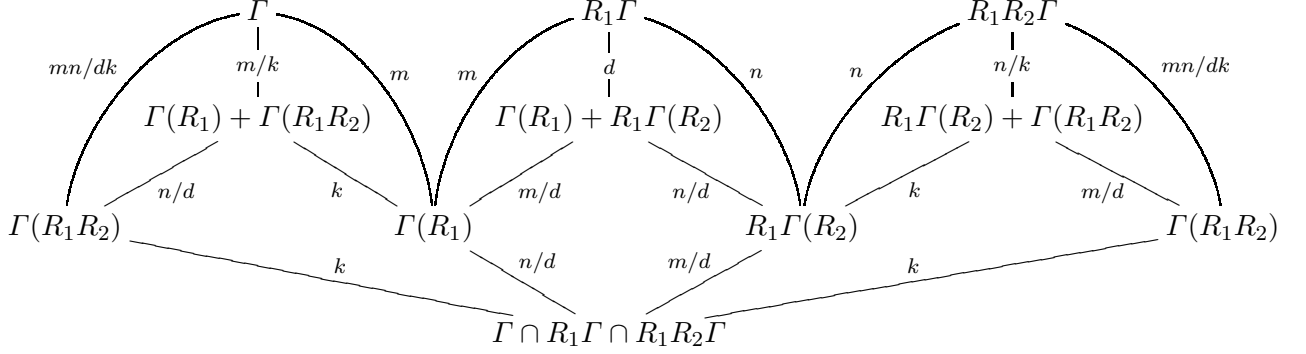


Figure 1. Relations between CSLs and their indices

We can even prove more:

Theorem 2. If $\Sigma(R_1)$ and $\Sigma(R_2)$ are coprime, then

$$\Sigma(R_1 R_2) = \Sigma(R_1) \Sigma(R_2). \quad (4)$$

Note that the condition that $\Sigma(R_1)$ and $\Sigma(R_2)$ are coprime is essential. In general we cannot expect equality. A simple counter example is given by $R_2 = R_1^{-1}$, if $\Sigma(R_1) > 1$, since $\Sigma(R_1) = \Sigma(R_1^{-1})$ holds in general [4] and $\Sigma(E) = 1$.

For m and n coprime the diagram in Fig. 1 simplifies considerably and the result is shown in Fig. 2.

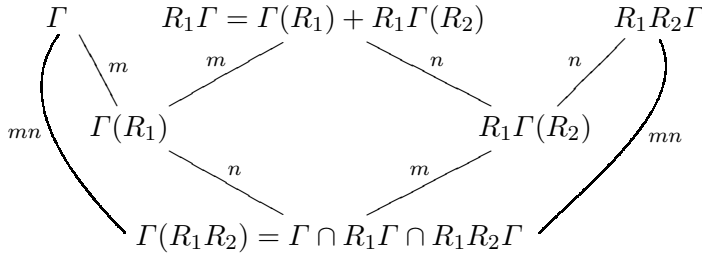


Figure 2. Relations between CSLs with $\Sigma(R_1)$ and $\Sigma(R_2)$ coprime

Moreover we can readily read off

Corollary 3. If $\Sigma(R_1)$ and $\Sigma(R_2)$ are coprime, then

$$\Gamma(R_1 R_2) = \Gamma \cap R_1 \Gamma \cap R_1 R_2 \Gamma = \Gamma(R_1) \cap R_1 \Gamma(R_2) \quad (5)$$

This result is rather technical but plays an important role in the following, since it relates $\Gamma(R_1 R_2)$ with some kind of multiple CSLs and provides the basis for something like a “prime decomposition” of CSLs.

Before we continue we want to point out that analogous results can be also obtained for similar sublattices, see e.g. [13]. There $\Sigma(R)$ has to be replaced by the corresponding index of the primitive similar sublattice, which is given by $\text{den}(R)^d$, where $\text{den}(R)$ is the denominator of the similarity rotation and d is the dimension. In fact, there is a close relationship between similar sublattices and CSLs, see [12, 14].

3. Multiplicity functions

We have already mentioned that the functions $f^{iso}(m)$ and $f(m)$ are in general not multiplicative. Nevertheless $f^{iso}(mn)$ (and likewise $f(mn)$) is not completely independent of $f^{iso}(m)$ and $f^{iso}(n)$. In fact we can prove [15]

Theorem 4. $f^{iso}(m)$ is supermultiplicative, i.e. $f^{iso}(mn) \geq f^{iso}(m)f^{iso}(n)$ if m and n are coprime.

The proof is mainly combinatorial and relies heavily on the multiplicativity of the index Σ as given in theorem 2. It is this theorem that guarantees that there are enough coincidence isometries of index mn .

Recall that $|\mathcal{P}|^{f^{iso}(m)}$ counts the number of coincidence isometries of index m . Correspondingly $f^{iso}(m)$ counts the number of distinct symmetry classes $R\mathcal{P}$ of coincidence isometries of index m , i.e. there exist exactly $f^{iso}(m)$ different cosets $R_i\mathcal{P}$ and every R with $\Sigma(R) = m$ is contained in exactly one of these cosets. Furthermore $f^{iso}(m)$ is an upper bound for the number $f(m)$ of CSLs of index m . In fact, all $R \in R_i\mathcal{P}$ generate the same CSL, and hence the set of all R that generate a given CSL is the union of finitely many cosets $R_i\mathcal{P}$. Let us denote the set of all coincidence isometries S that generate the CSL $\Gamma(R)$ by $\mathcal{S}(R)$. Clearly there are exactly $f(m)$ different $\mathcal{S}(R_j)$ with index m . The fact that $\mathcal{S}(R)$ consists of more than one symmetry class $R\mathcal{P}$ in general makes the determination of $f(m)$ more difficult than the computation of $f^{iso}(m)$ and in general the expressions for $f(m)$ are more complicated than those for $f^{iso}(m)$, see [10, 11] for examples. Nevertheless we can show

Theorem 5. $f(m)$ is supermultiplicative, i.e. $f(mn) \geq f(m)f(n)$ if m and n are coprime.

The proof is again combinatorial, though slightly more difficult. In fact one needs the following lemma, which is also interesting on its own:

Lemma 6. Assume that $\Sigma(R) =: m$ and $\Sigma(S) =: n$ are coprime. Then

$$n\Gamma \cap \Gamma(RS) = n\Gamma(R) \quad \text{and} \quad mR\Gamma \cap \Gamma(RS) = nR\Gamma(S). \quad (6)$$

This lemma does not only tell us that we can recover $\Gamma(R)$ and $\Gamma(S)$ from $\Gamma(RS)$ alone but it also tells us how to do so: just by taking the intersection of $\Gamma(RS)$ with a suitable similar sublattice of Γ .

Multiplicativity can be destroyed for several reasons, and we can read them off from this lemma. First, there may be isometries Q of index $\Sigma(RS) = mn$ that cannot be written as a product $Q = RS$ with $\Sigma(R) = m$ and $\Sigma(S) = n$. As an example we mention $\Gamma = 2\mathbb{Z} \times 3\mathbb{Z}$. Here $f^{iso}(6) = f(6) = 1$, but $f^{iso}(2) = f(2) = 0 = f^{iso}(3) = f(3)$. Further examples can be found in [16].

Secondly, two isometries R, R' that generate the same CSL $\Gamma(R) = \Gamma(R')$ might give rise to different CSLs $\Gamma(RS)$ and $\Gamma(R'S)$. This is no problem as long as R and R' are symmetry related. In this case the set $\{\Gamma(R'S_k)\}_{k=1}^{f(n)}$ is just a permutation of $\{\Gamma(RS_k)\}_{k=1}^{f(n)}$, where S_k runs over a complete set of not symmetry related S_k of index $\Sigma(S_k) = n$. However, if R and R' are not symmetry related additional CSLs might occur.

Analogous results hold for similar sublattices. Let $g(m)$ be the number of similar sublattices of index m . Then the function $g(m)$ is in general only supermultiplicative. An example for a lattice with non-multiplicative $g(m)$ is again the lattice $\Gamma = 2\mathbb{Z} \times 3\mathbb{Z}$. But note that similar sublattices seem to be more sensitive to violation of multiplicativity than CSLs. E.g., for $\Gamma = \mathbb{Z} \times 5\mathbb{Z}$ multiplicativity is violated for $g(m)$ while $f(m)$ is still multiplicative [16, 17].

4. A criterion for multiplicativity

We have seen that $f(m)$ and $f^{iso}(m)$ are in general only supermultiplicative. Now the interesting question is whether there exist some criteria for multiplicativity and the answer is positive. A first hint is given by known examples in $d \leq 4$. For root lattices in $d \leq 4$ the multiplicity functions $f(m)$ and $f^{iso}(m)$ are usually multiplicative. The reason is that these lattices are related to principal ideal domains (and thus unique factorization domains) of algebraic integers or quaternions. So we expect that some kind of unique factorization property is essential. In fact we can prove

Theorem 7. *The following statements are equivalent:*

- (i) $f(m)$ is multiplicative.
- (ii) Every (ordinary) CSL $\Gamma(R)$ can be written (uniquely) as $\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$, where the indices $\Sigma(R_i)$ are powers of distinct primes.
- (iii) Every MCSL $\Gamma(R_1, \dots, R_n)$ of order n can be written (uniquely) as $\Gamma(R_1, \dots, R_n) = \Gamma_1 \cap \dots \cap \Gamma_k$, where the Γ_k are MCSLs of order at most n and whose indices Σ_k are powers of distinct primes.

Note that Lemma 6 guarantees the uniqueness of the decomposition $\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$, if it exists. Lemma 6 is also the main ingredient for the proof, which again also involves combinatorial arguments. But be careful. The decomposition $\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$ does not imply the decomposition $R = R_1 \cdots R_n$, in general R is not even symmetry related to $R_1 \cdots R_n$. The situation is even worse. If $R = R_1 \cdots R_n$ is a decomposition of R then in general $\Gamma(R) \neq \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$, which is due to the fact that $O(n)$ is not Abelian for $n \geq 2$.

A corresponding criterion for the coincidence isometries exists as well. The formulation of it is a bit more intricate, since isometries usually do not commute. For CSLs the decomposition into its prime power constituents is unique (up to permutation), for isometries a decomposition will depend strongly on how the factors are ordered.

First notice that if the coincidence isometry R with $\Sigma(R) = mn$ can be factored as $R = R_1 R_2$ with $\Sigma(R_1) = m$ and $\Sigma(R_2) = n$ coprime, then R_1 and R_2 are uniquely determined up to elements of the point group \mathcal{P} , i.e. all other decompositions are of the form $R = (R_1 Q)(Q^{-1} R_2)$ with $Q \in \mathcal{P}$. Note that R_2 and $Q^{-1} R_2$ are usually not symmetry related, whereas R_1 and $R_1 Q$ are.

At this point it is not clear whether the existence of a decomposition $R = R_1 R_2$ implies a decomposition $R = R'_2 R'_1$, where $\Sigma(R_1) = \Sigma(R'_1) = m$ and $\Sigma(R_2) = \Sigma(R'_2) = n$. This motivates the following definitions: We call a bijection $\pi = \{p_1, p_2, \dots\}$ from the positive integers onto the prime numbers an ordering of the prime numbers. We call a decomposition of a coincidence isometry $R = R_1 \cdots R_n$ a π -decomposition of R if $\Sigma(R_i)$ is a power of p_i for any i (we allow $\Sigma(R_i) = p_i^0 = 1$). It is clear that any π -decomposition can be unique only up to point group elements.

We can now formulate the analogue of theorem 7 for $f^{iso}(m)$

Theorem 8. *The following statements are equivalent:*

- (i) $f^{iso}(m)$ is multiplicative.
- (ii) There exists an ordering π of the prime numbers such that any coincidence isometry R has a (unique) π -decomposition.
- (iii) For any ordering π of the prime numbers there exists a π -decomposition of every coincidence isometry R .

Given these two quite similar criteria we may expect that there is some connection between the multiplicativity of $f(m)$ and $f^{iso}(m)$. In fact we can prove

Theorem 9. *$f(m)$ is multiplicative if $f^{iso}(m)$ is.*

Here it is worth to comment on the various decompositions that occur here. For simplicity we assume that only two prime powers are involved, say $\Sigma(R) = p_1^{r_1} p_2^{r_2}$. Then the multiplicativity of $f^{iso}(m)$ guarantees the existence of two decompositions $R = R_1 S_1$ and $R = R_2 S_2$ with $\Sigma(R_1) = p_1^{r_1} = \Sigma(S_2)$ and $\Sigma(R_2) = p_2^{r_2} = \Sigma(S_1)$. In this case the unique decomposition of $\Gamma(R)$ reads $\Gamma(R) = \Gamma(R_1) \cap \Gamma(R_2)$. So given the decompositions of R we get immediately the decomposition of $\Gamma(R)$. However, it does not work the other way round. So given a decomposition of $\Gamma(R)$ we do not get any information on the decompositions of R , even if we would know that they exist.

Now what about the converse of theorem 9? Does it exist? We do not know the answer so far. So we conclude with an open question: Does the multiplicativity of $f(m)$ imply the multiplicativity of $f^{iso}(m)$? Or are there lattices with multiplicative $f(m)$ but non-multiplicative $f^{iso}(m)$?

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